Development of Thermal Runaway Risk Database

- Data Collection and AI for Safety Database in Partnership with Sandia

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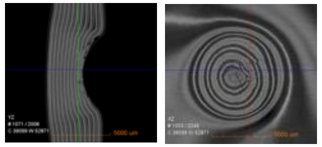
Sandia National Laboratory

Battery Pack

Battery Modules

Battery Cells



XCT: Indented Battery

Project Overview

- To develop a Li-ion battery thermal runaway risk database for energy storage systems
- To understand and manage the safety risks of Li-ion batteries in energy storage systems, especially for thermal runaway
- This work fits specifically into OE efforts to ensure a resilient, reliable, and flexible electricity system

Ultimate Goal: Select a Li-ion cell with unknown safety risk; perform a single indentation test; use the database and machine learning prediction tools to rank/predict the cell's thermal runaway risk

Thermal Runaway Risk Database Development

- **Project Period:** FY18-FY21 (actual start in June 2018)
- **Annual Budget:** $300K (ORNL)
- **Project Team:** Collaboration with Sandia National Laboratory (Loraine Torres-Castro, Yuliya Preger and Josh Lamb)
- **Project Milestones:**
  - Complete 10 Ah NMC cells and 10 Ah LFP cells testing at ORNL and Sandia
  - Web-based database development hosted by Sandia
  - Data Analysis: Thermal signature analysis using infrared imaging
  - Data analyzed using machine learning tools: Basic and advanced

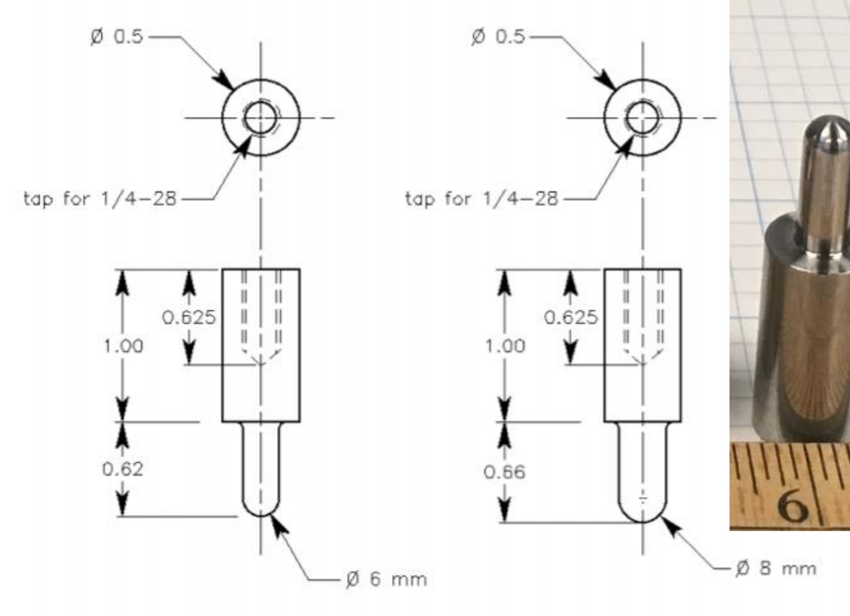
Updated ORNL-Sandia Test Procedures and Standards

Internal Short-ciruit Induced Thermal Runaway

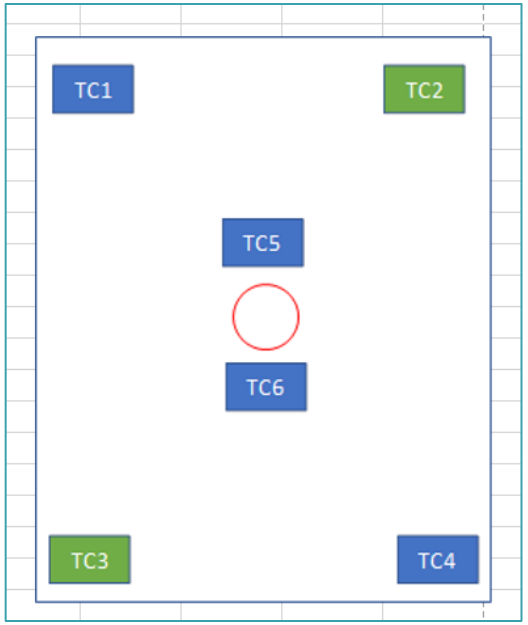
- Mechanical abuse (indentation)

Updated Test Protocols:

- Cycle cell 5 times at C/2 between 3.0-4.2V to determine SOC and discharge to test SOC
- Hydraulic or servo-motor driven load frame
- 6 mm punch (most sensitive, small contact)
- 0.05 inch per minute compressive loading
- 25 mV V_{oc} drop
- Hold the punch after short circuit
- Temperature measurement:
  - 5 mm from the indenter
  - At cell corners when possible



Punches for Battery Testing		
ELC-2019.03.001	Scale: 1.5:1	
Dimensions: inches (unless otherwise specified)	Material: stainless steel	
Make four (4) pieces of each		
Edgar Lara-Curzio	ORNL	March 2019



Thermocouple Locations on Large-format Cells

Select the most sensitive test to allow safety risk ranking

Li-ion Cells: Disassembled EVs and Commercial Sources

Large-format Prismatic Cells Tested at ORNL and Sandia

2017 Chevy VOLT (26 Ah)

2013 Nissan Leaf (33 Ah)

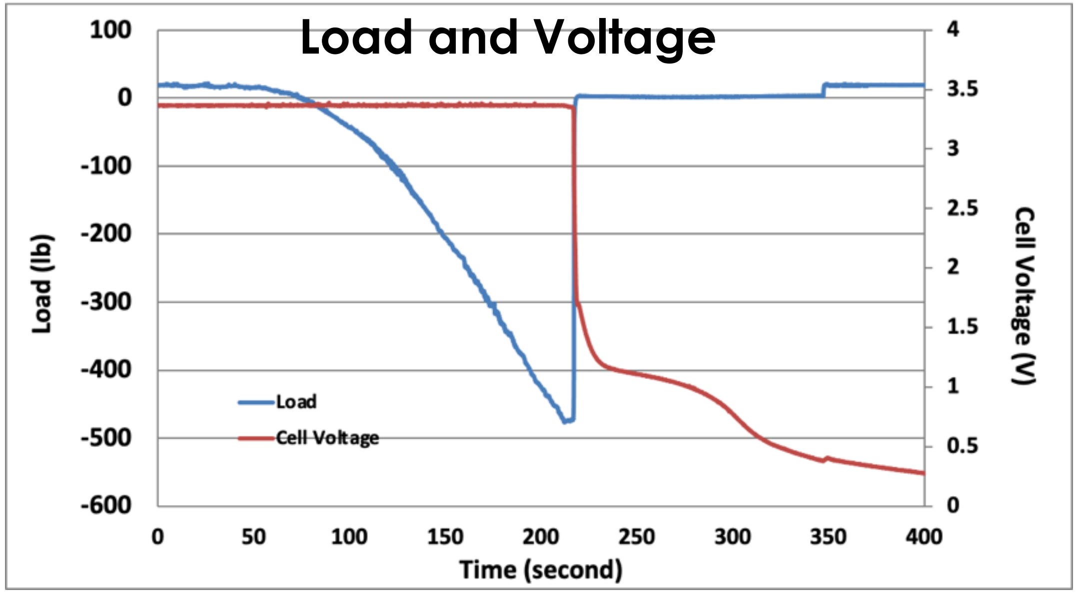
Commercial NMC Cells (10 Ah)

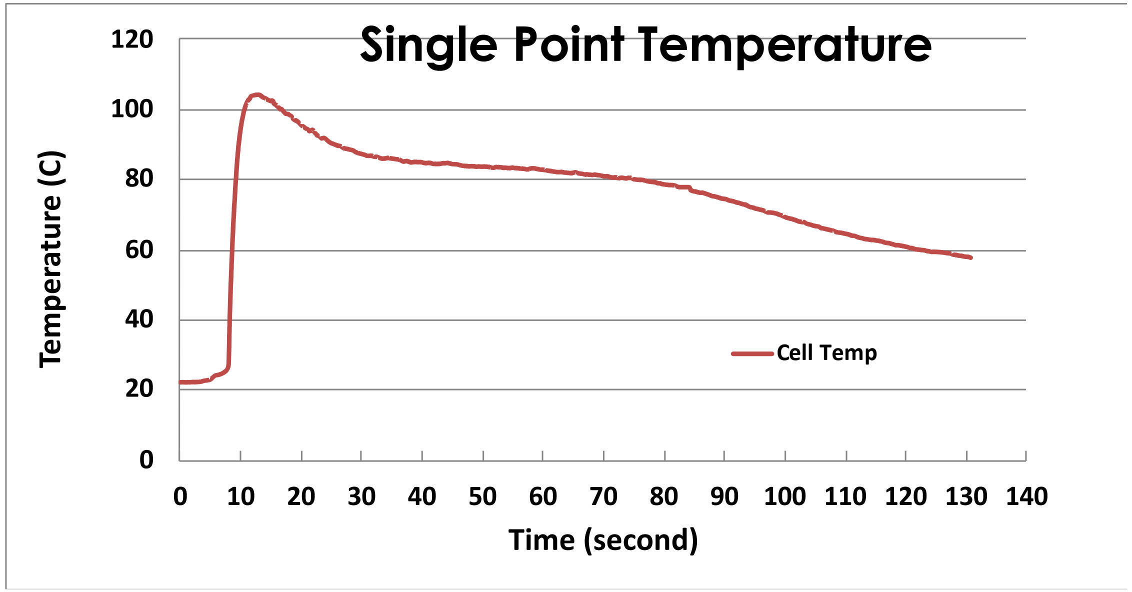
Commercial LFP Cells (10 Ah)

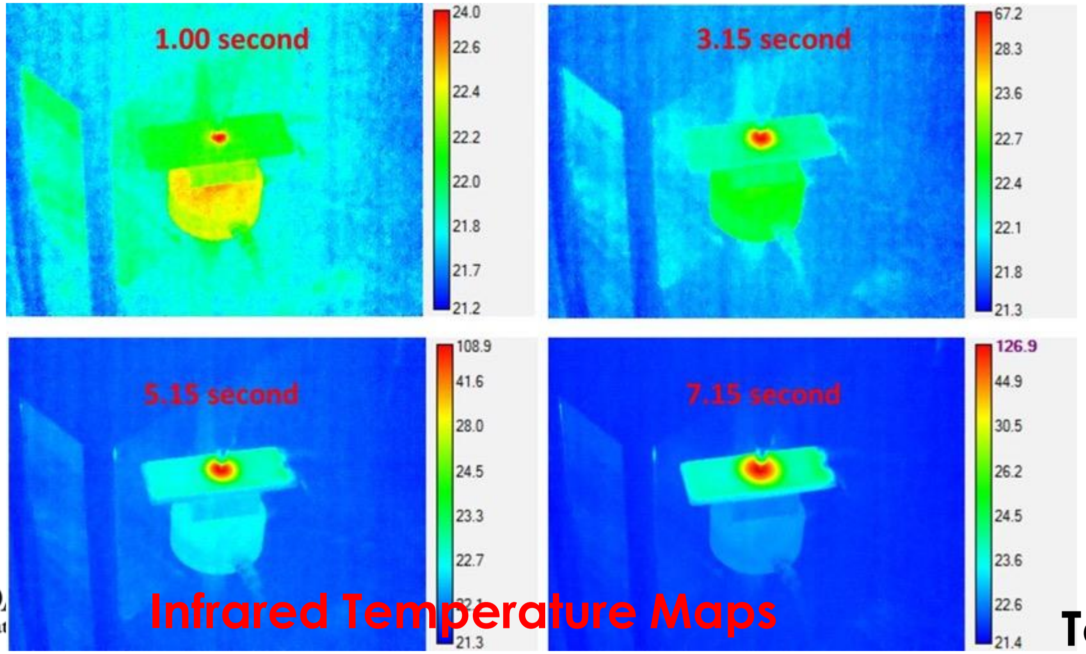
10 NMC Cells (5 SOC x 2) after Testing
Left to right: 0% SOC -> 100% SOC

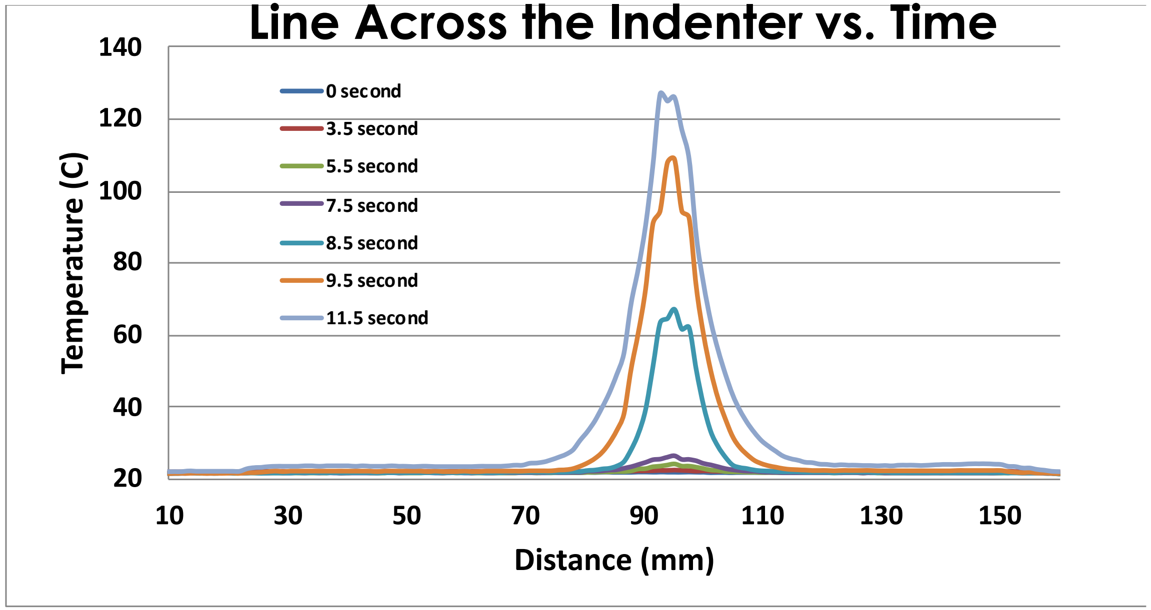
10 LFP Cells (5 SOC x 2) after Testing
Left to right: 0% SOC -> 100% SOC

Test Data Analysis: Thermocouple vs. IR Imaging



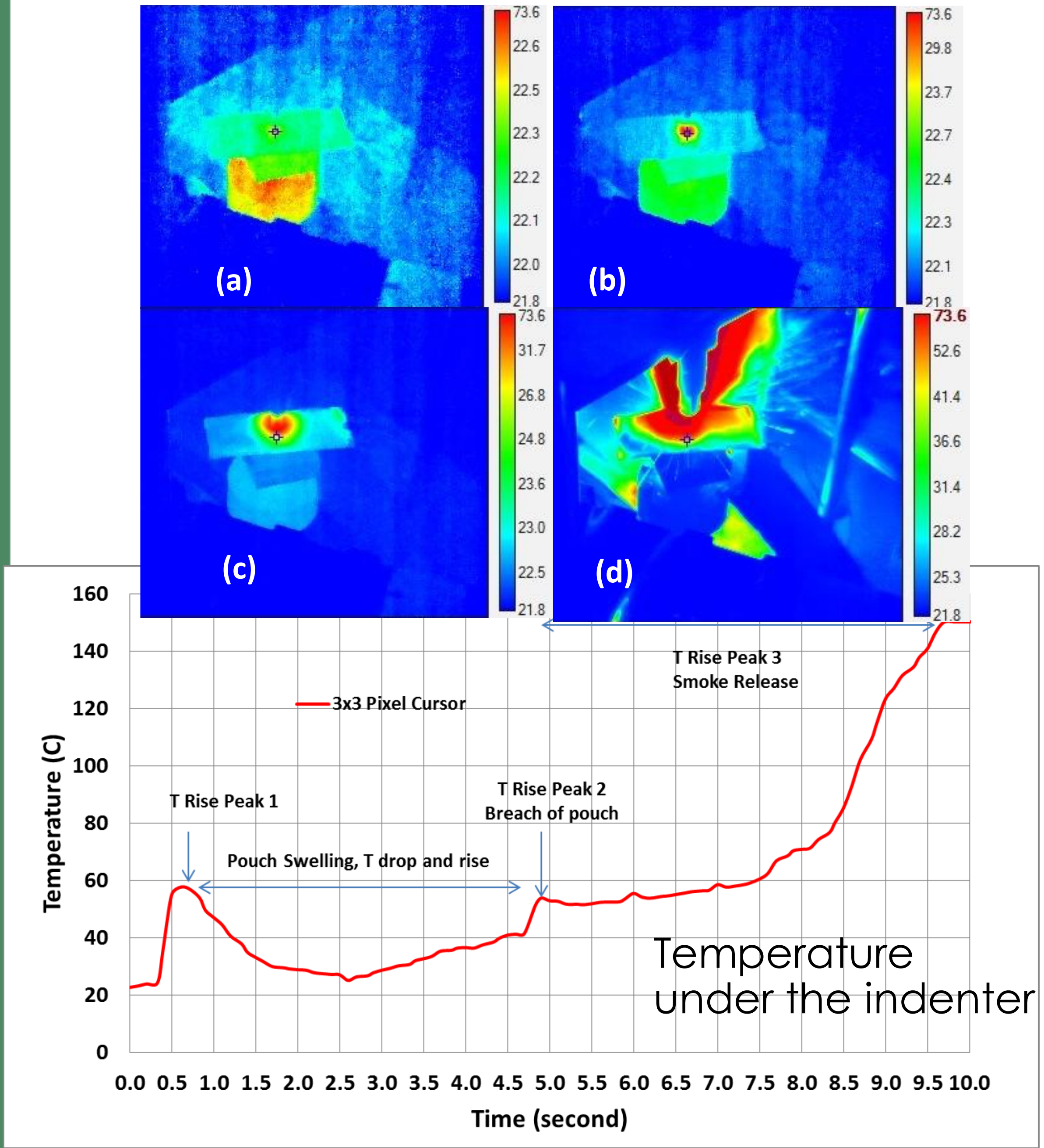




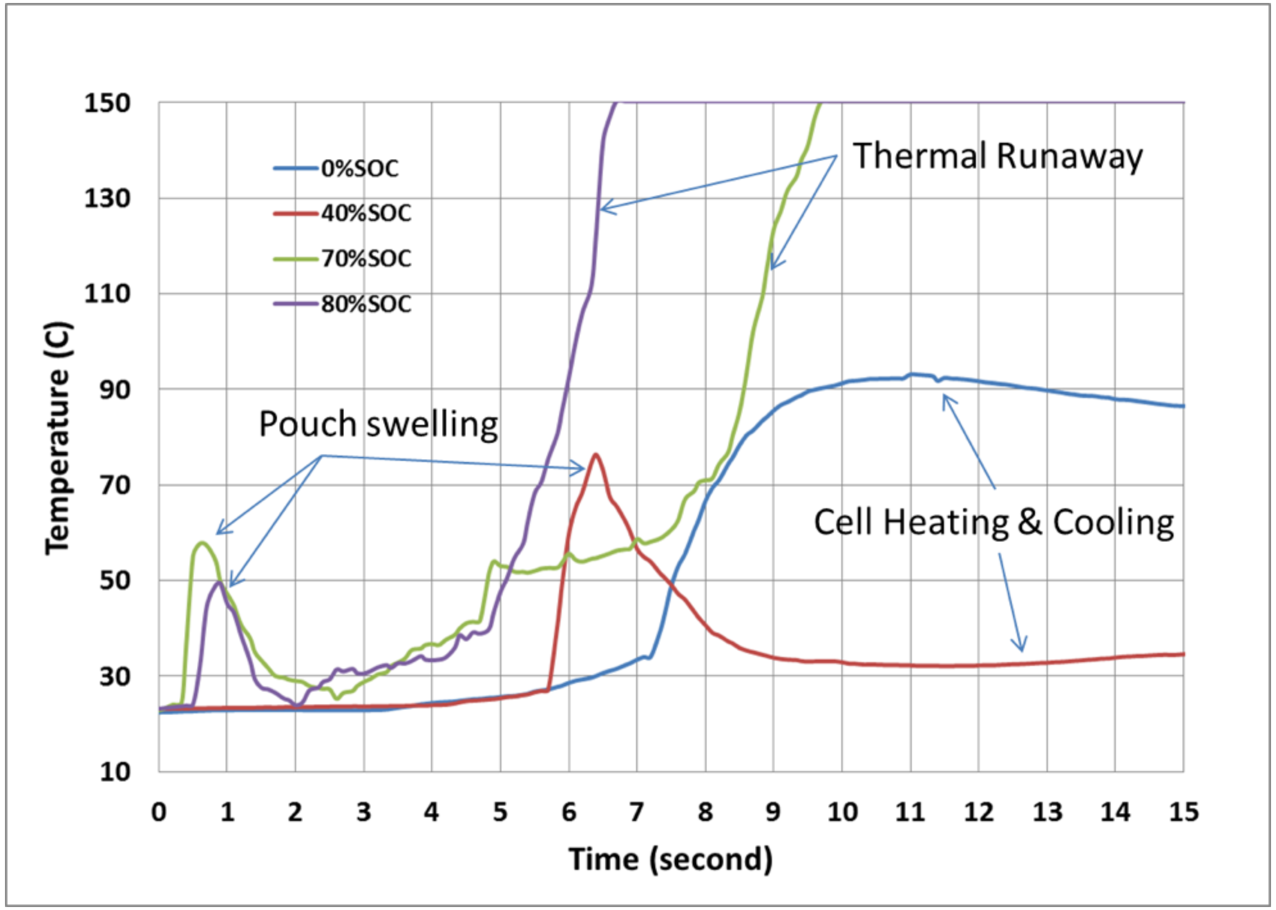


Temperatures values sensitive to thermocouple location

Thermal Signatures of Thermal Runaway Cells



Temperature under the indenter

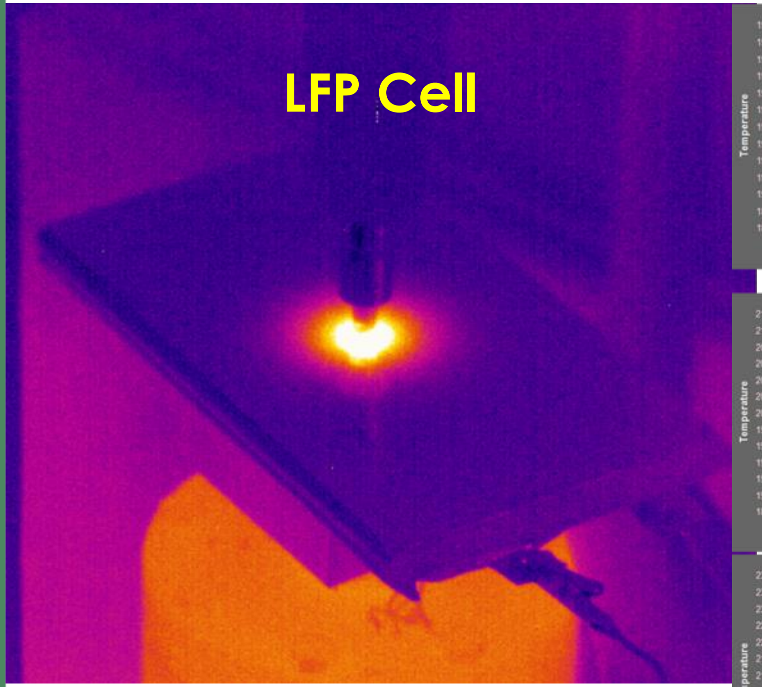


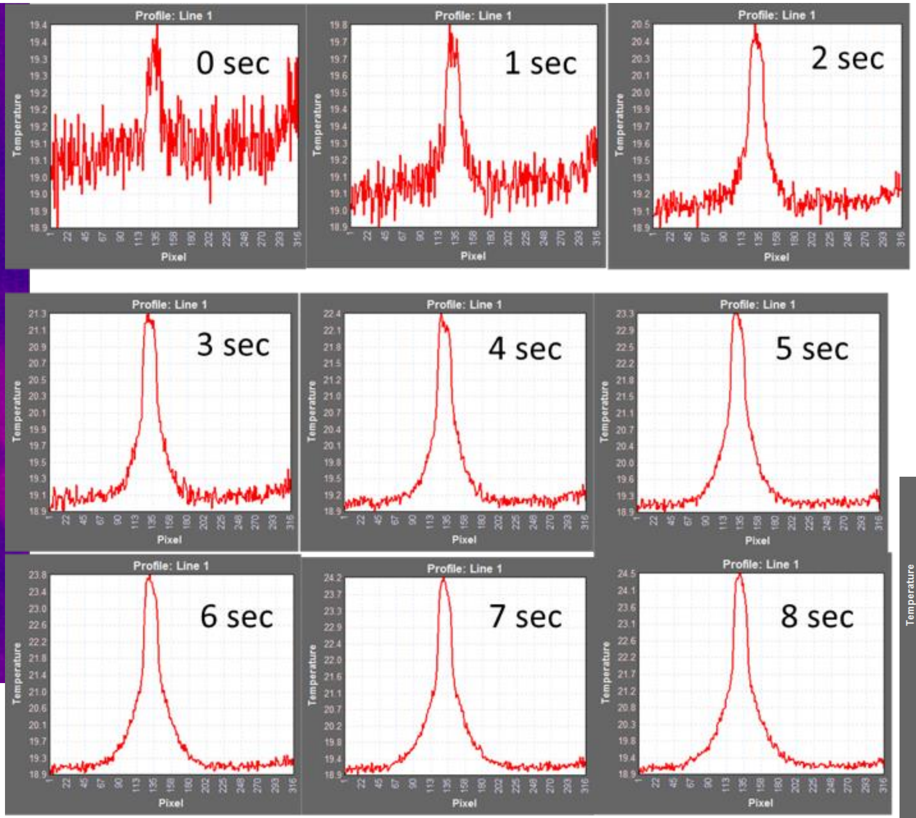
Thermal Signatures from IR imaging:

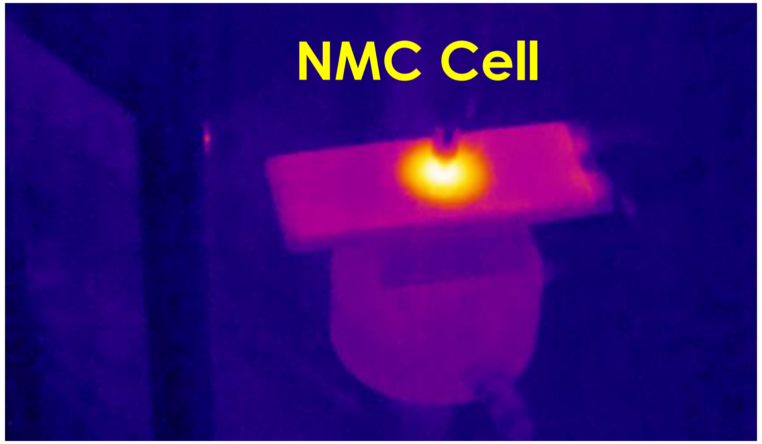
- Pouch swelling (sharp peak and time stamp)
- Temperature rise > 150°C, timing, slope
- Over-all temperature curve vs. Time

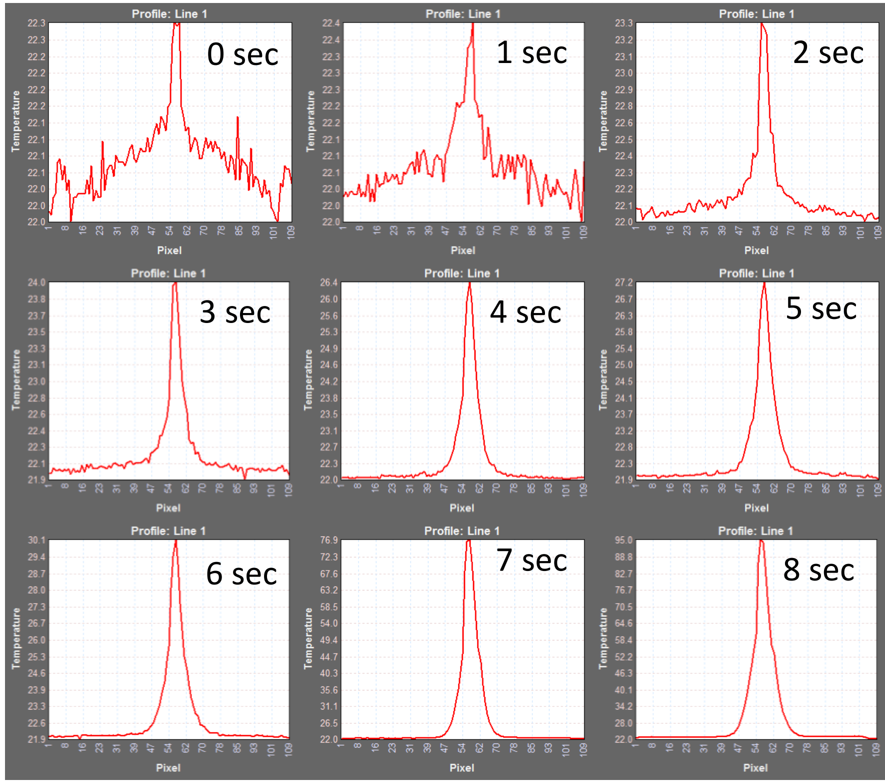
Key observation: 40% SOC cell did not go to thermal Runaway. The pouch swelling peak indicated high risk

Thermal Signatures NMC Cells vs. LFP Cells (10 Ahr)



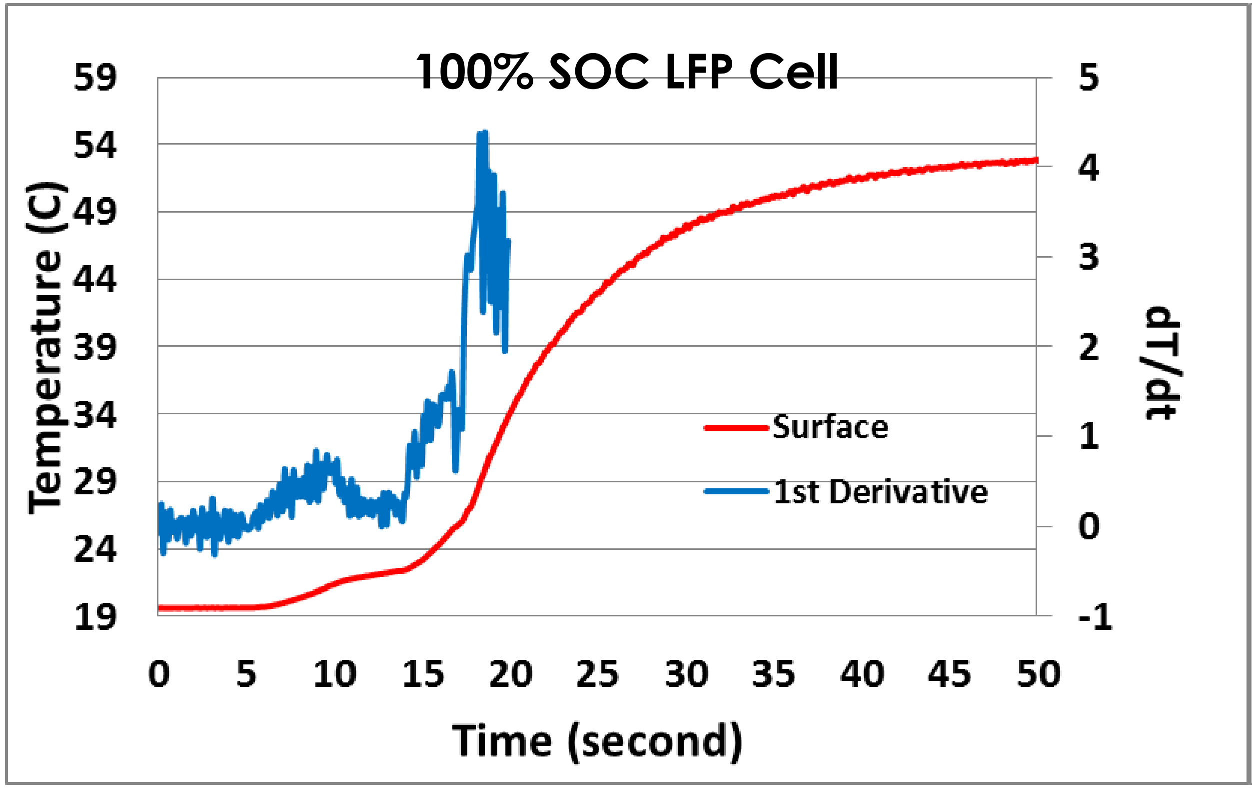


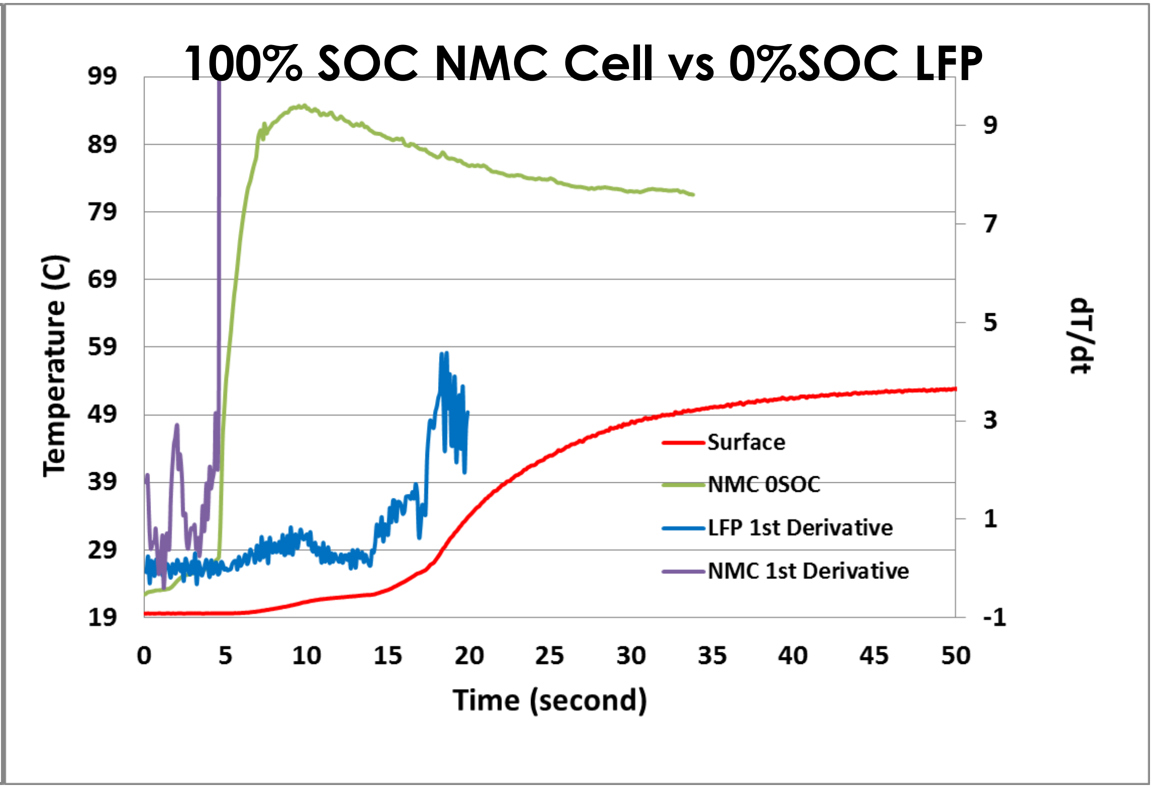




- **Both cells did not go to thermal runaway**
- **IR line profiles provided more thermal signatures**
  - Peak temperature
  - Peak width at half maximum
  - Area under the peak
  - Shape of the peaks (symmetry)

Thermal Signature: Temperature Rise Curves - 0%SOC NMC vs 100%SOC LFP





100% LFP:
Maximum temperature rise: 54°C at 50 second
1st derivative maximum: 4°C/sec @ 20 second

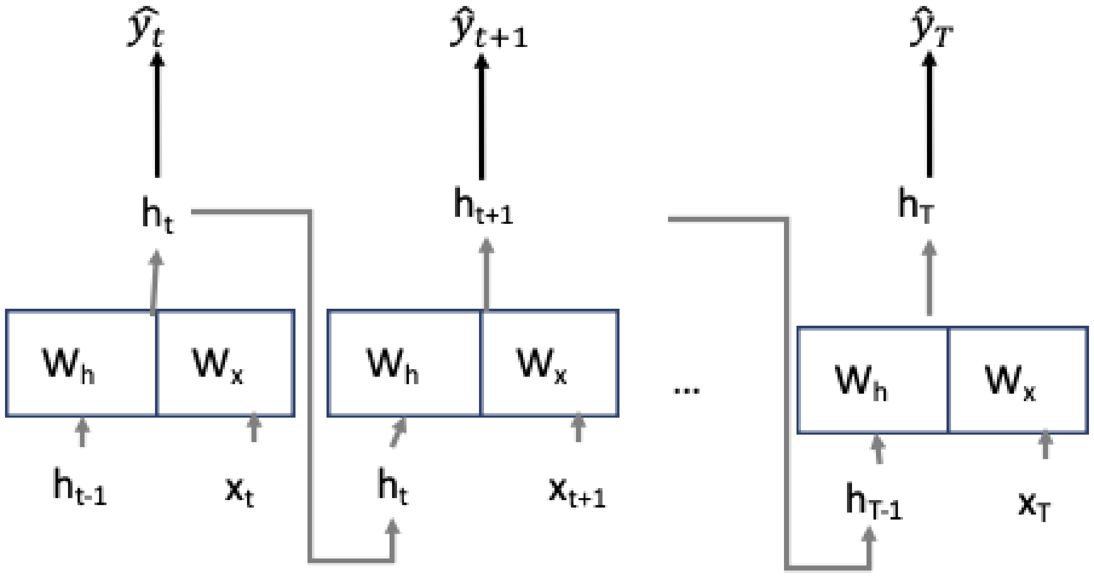
Thermal runaway risk score: 0 (low risk)

100% NMC:
Maximum temperature rise: 94°C at 10 second
1st derivative maximum: >10°C/sec @ 10 second

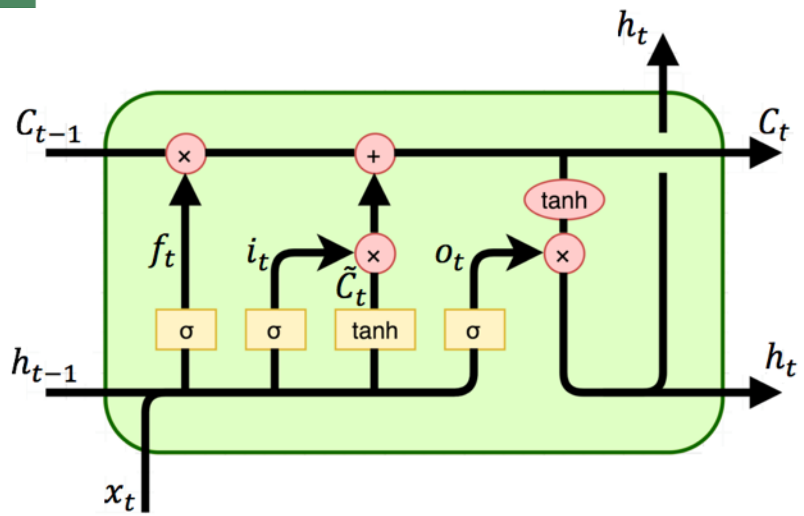
Thermal runaway risk score: 100 (high risk)

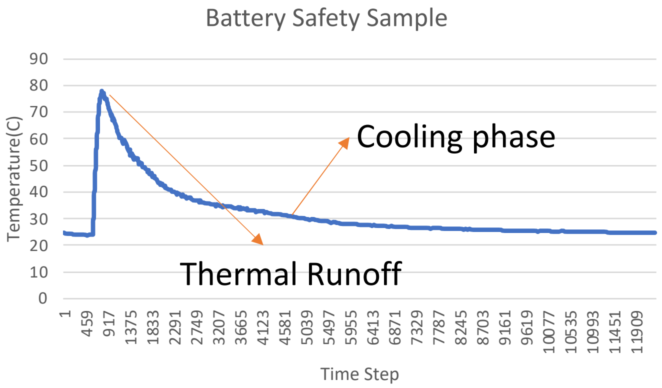
TR Risk Database: human observation to machine learning and pattern recognition

Database Tool: Advanced ML models to predict the temporal response of battery critical parameters during safety events



Sequence Learners





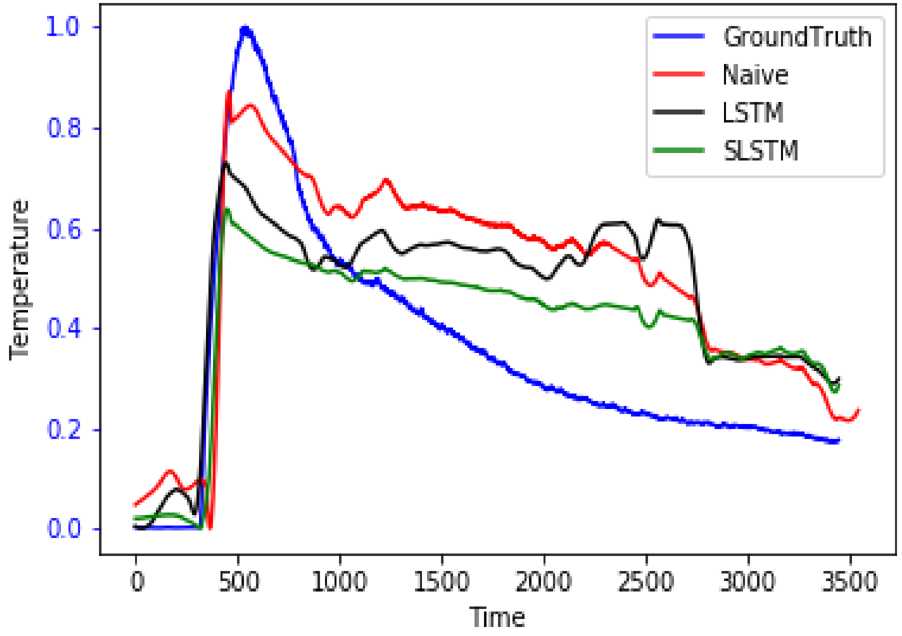
- Different aspects battery predictions like safety and ageing require short-range and long-range temporal characterizations respectively. Next few slides we study ML models based on time period of interest.
- Multivariate observations such as Voltage, Load and Temperature are labeled for total time. These continuous observations are broken into timesteps with an appropriate window size
- LSTM is a variant of sequence learner that allows it to easily "memorize"' information for an extended number of timesteps. The "long term"' memory is stored in a vector of *memory cells*
- RNN (recurrent neural network) are best suited for time series data collected from experiment.

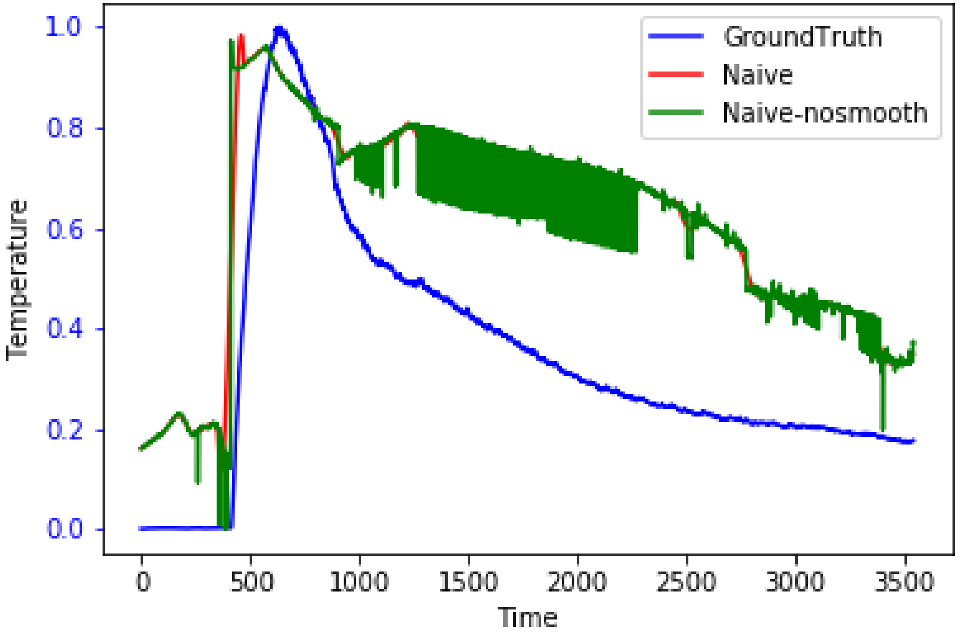
Kannan R., Graves. J.A., Wang H., Allu S., "Novel sequence model for characterization of Battery predictions", SIAM Data Mining, 2021

ML modeling for Battery Thermal Runaway Risks

- Models
  - Local Models – Any ‘b’ bandwidth information (voltage, load) can determine a temperature in the next ‘k’ seconds
    - Advantages – Can augment and integrate experiments of different resolution and from d
    - Disadvantage – Cannot capture the global properties of one peak point and monotonically decreasing cooling phase.
  - Global Models – Every time step ‘t’ is determined by the entire [1,..t-k] information (voltage, load)
    - Disadvantage – (a) Very expensive experiment and fewer samples (only 34 samples). Cannot generalize well for out of samples scenarios. (b) all the experimental data will be normalized as if conducted with similar settings.
  - Our proposed hybrid method – After every epoch of local models, test the model on a global hold out sample.
- Scientific Constraints
  - Unimodal Isotonic – Single peak and monotonically reduces after the peak
  - Savitzky-Golay Smoothing to alleviate local oscillations

Performance of Global ML models (training of initial dataset)

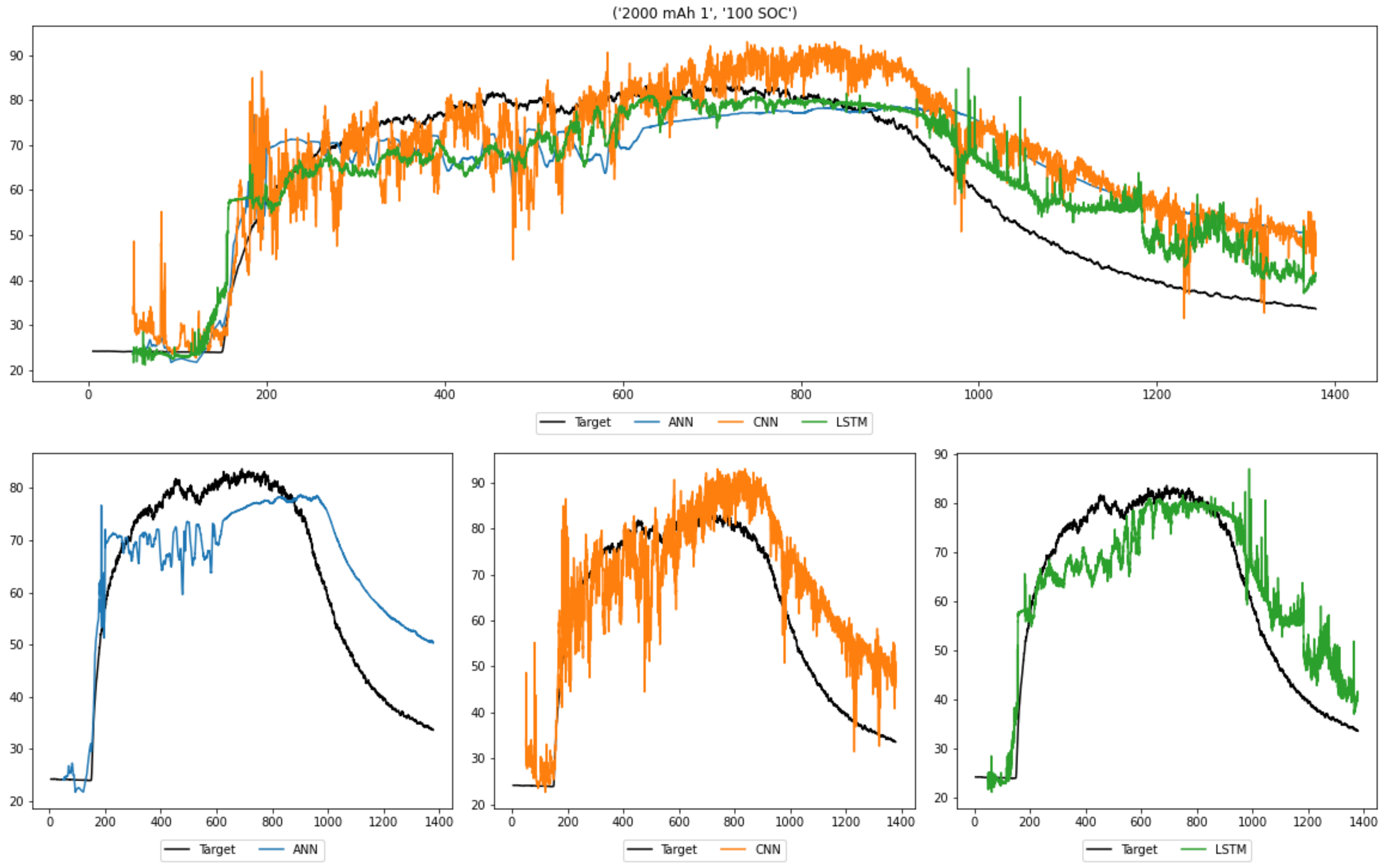




Initial ML data analysis on small cells in FY20 have been updated

- A mini-batch training of size 13 and three layers of LSTM was chosen. Since there were 39 training points, a batch size of 13 gave sufficient randomization without replacement.
- We are using Mean Square Error $\frac{1}{n}\sum_{i=0}^{n}\sum_{t}(y_t - \hat{y}_t)^2$ to represent the closeness of the ground truth temperature with the predicted temperature.
- We plot the temperature curves across the different variants *naïve, LSTM* and *SLSTM.* All the three variants were good in capturing the thermal run away. But they were differing in the max temperature and the decaying temperature

Performance of Local ML model (training of initial dataset): Thermocouple data from Chevy VOLT Cells



- Consider every [1..b] bandwidth information to predict temperature after 'k' steps into the future.
- Every sample is 300 length with a sequence of 150 using voltage and load to predict the temperature.
- In order to reduce the oscillations in the local model, we use isotonic regression and Savitzky-Golay as post-processing step.

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Database Interface: Display Original Cell Abuse Data and Combine Information from Different Datasets

Sandia Hosting Thermal Runaway Risk Database

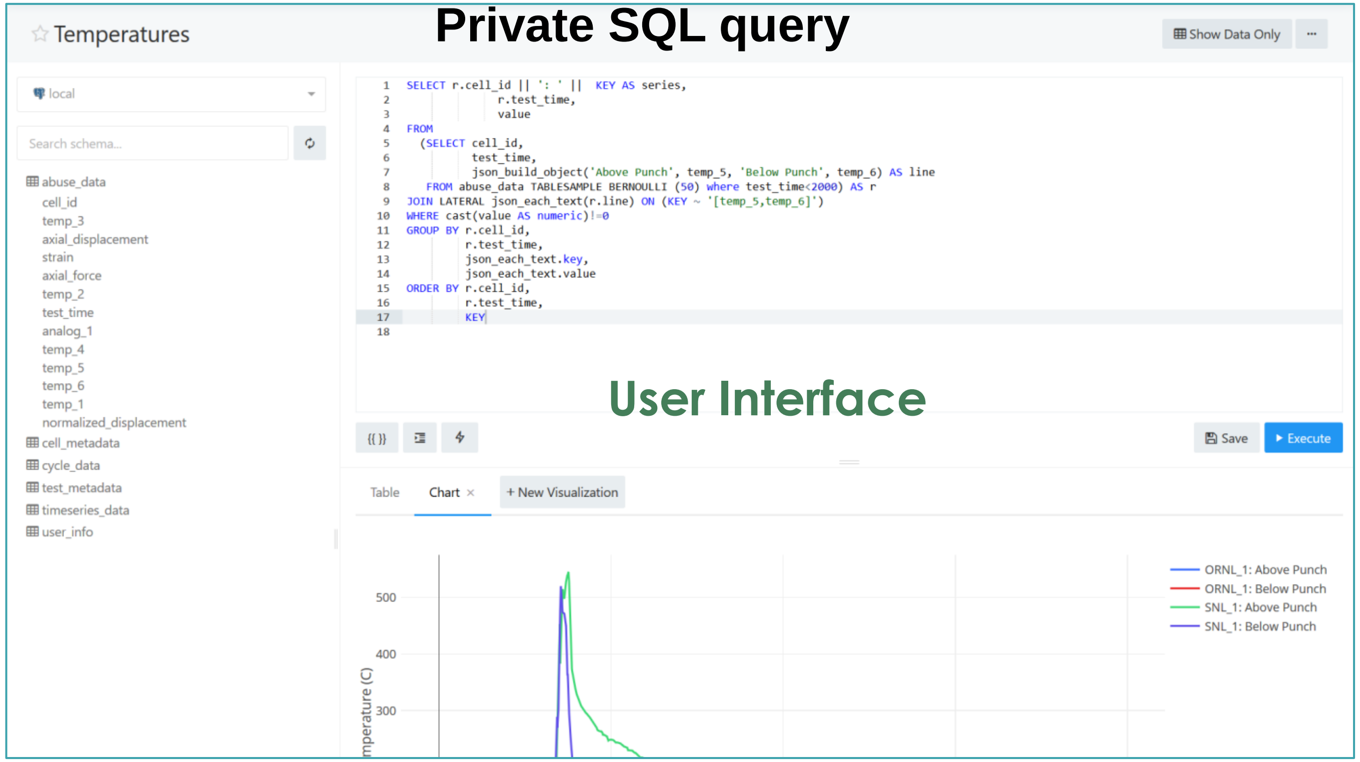
- Uses the same functionality developed to import and display cycling data in batteryarchive.org
- Original abuse data is imported in a Postgres database using Python scripts
- New quantities can be calculated
- Data can be queried using SQL queries, displayed in tables, or exported in JSON format
- Data filtering by metadata is available

Database Functions:

- Host test data submitted by labs and users
- General query and thermal runaway risk ranking
- Plot data and compare test results
- Advanced analysis:
  - ➢ Thermal and mechanical signatures
  - ➢ Machine learning analysis
  - ➢ Compare single entry to database and relative risk ranking

Data Entries and Format:

- Cell metadata
  - ➢ Dimension, mass
  - ➢ Chemistry: cathode, anode
- Test Data:
  - ➢ Cell voltage, displacement
  - ➢ Applied load
  - ➢ Temperatures
- Data in .csv and Excel Spreadsheets



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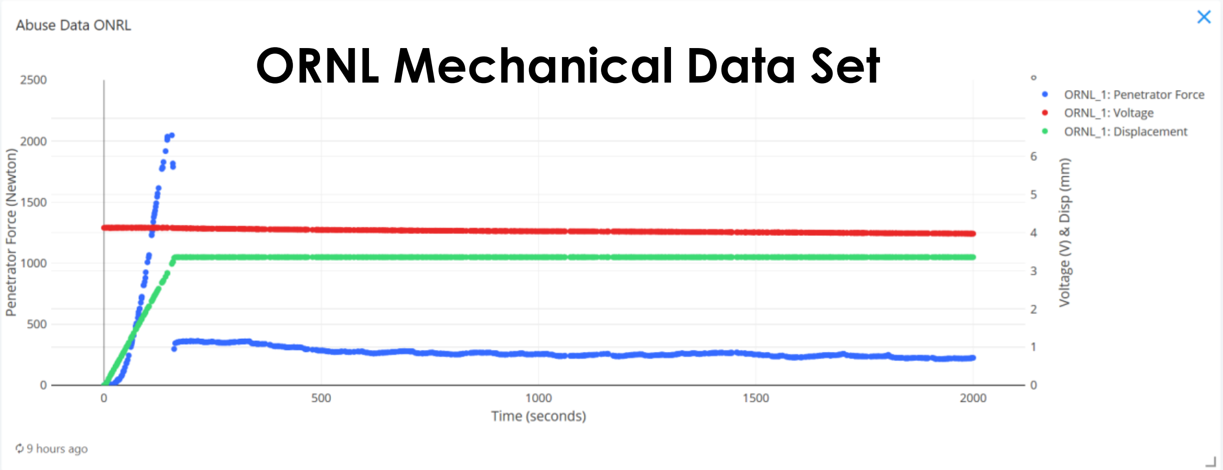
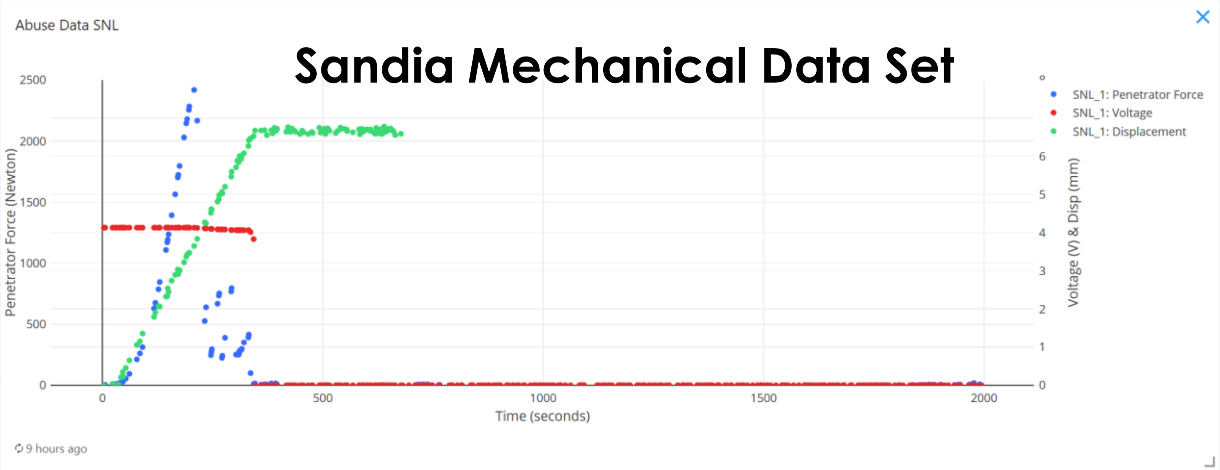
Example: Display Original Data & Combine Information From Different Datasets on Web Dashboards

2017 Chevy VOLT Cells at Sandia and ORNL
No thermal runaway for SOC <100% in both labs and different results in 100% SOC

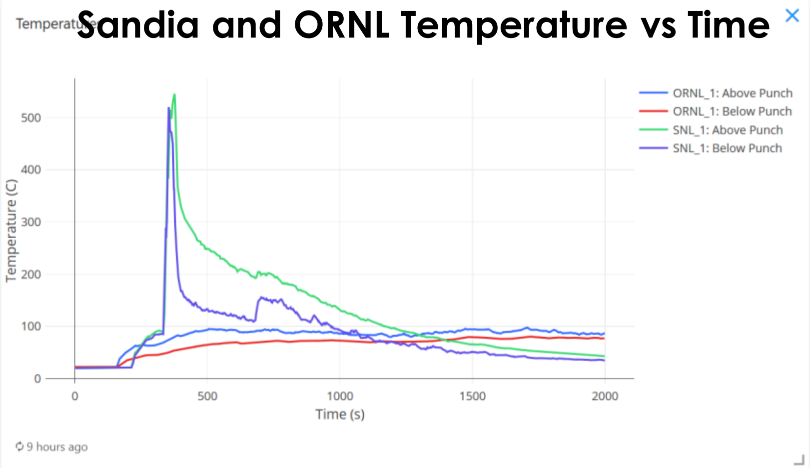
ORNL Mechanical Data Set



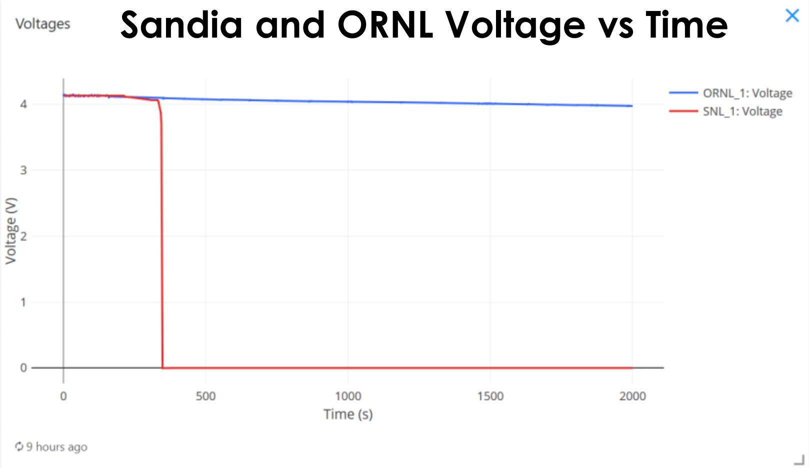
Sandia Mechanical Data Set



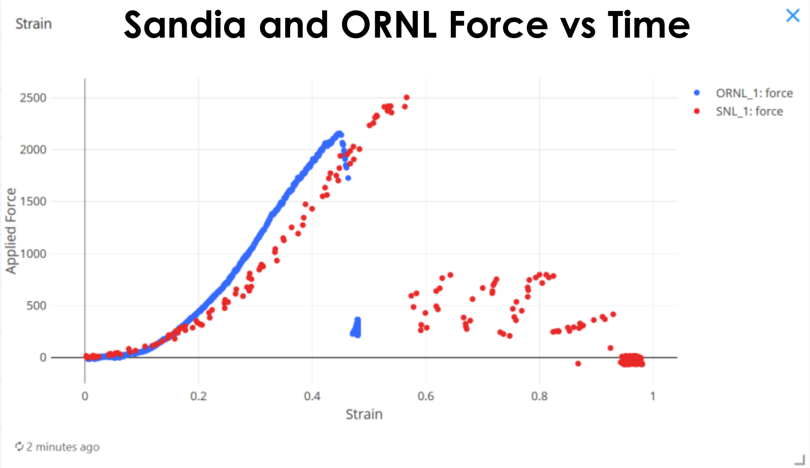
Sandia and ORNL Temperature vs Time



Sandia and ORNL Voltage vs Time



Sandia and ORNL Force vs Time



Test Systems:
- ORNL: Servo motor driven
- Sandia: Hydraulic load frame

Comparison on 100% SOC Cells:
- ORNL: No thermal runaway
- Sandia: Thermal runaway

In-depth Analysis: Test Sensitivity
- Stopping and holding mechanisms are different for the two systems
- Small displacement uncertainty can result in different responses

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Summary and Future Plan

FY2021:

- Cell Testing:
  - ✓ Completed 10 Ah NMC cells testing at ORNL and Sandia
  - ✓ Completed 10 Ah LFP cells testing at ORNL and Sandia
  - ✓ 5 Ahr NMC and LFP cells purchased/started
- Utilized infrared imaging data to analyze thermal signature during indentation tests
- Machining learning (ML) tools developed at ORNL
- Database interface developed at Sandia with initial inputs and basic functions
- Other accomplishments/publications:
  - ✓ Two publications
  - ✓ Two invited talks

FY 2022 Plan:

- Continue working with Sandia on database development and refinement of test procedures
- Continue cell testing and data collections:
  - Low and medium capacities cells
  - More cell chemistry: LFP, NMC
- ML/AI tool development
- Sandia web interface to host test data and user analysis functions
- Standardization: UL and ESS test code
- Education: Communicate with ESS and cell manufacturers on test method and results

Acknowledgement

Support of DOE Office of Electricity (Dr. Imre Gyuk)

ORNL Program Management: Tom King and Michael Starke

Publications:

1. Zhenpo Wang, Shiqi Xu, Xiaoqing Zhu, Hsin Wang, Lvwei Huang, Jing Yuan, Weiqiang Yang, "Effects of short-term over-discharge cycling on the performance of commercial 21,700 lithium-ion cells and the identification of degradation modes", Journal of Energy Storage, Vol. 35 p102257 (2021)

2. Zhenpo Wang, Jing Yuan, Xiaoqing Zhu, Hsin Wang, Lvwei Huang, Yituo Wang, Shiqi Xu, "Overcharge-to-thermal-runaway behavior and safety assessment of commercial lithium-ion cells with different cathode materials: A comparison study", Journal of Energy Chemistry, Vol. 55, pp484-498 (2021)

Two Invited Talks: Hsin Wang

1) Invited Speaker: April 21, 2021, 2021 DOE Energy Storage Reliability and Safety Forum, organized by Sandia National Laboratory. Title: "Internal short circuit induced thermal runaway" and panelist in battery safety.

2) Invited Speaker and Panelist: June 29 - 30, 2021, The Battery Safety Summit. Title: Mechanically Induced Internal Short Circuit and Thermal Runaway in Li-Ion Batteries